

## AUTHOR INDEX TO VOLUME 141

Aguilar, A., see R. Sayós	141 (1990) 401
Anderson, M.R., see A.E. Russell	141 (1990) 41
Badiali, J.P. and F. Forstmann, Long-range correlation between polar molecules adsorbed onto a dielectric solid	141 (1990) 63
Balter, A., see O. Rolinski	141 (1990) 265
Baňácký, P., Effective two-level reduction of <i>N</i> -level system dissipative quantum dynamics	141 (1990) 249
Bertrán, J., see M.N.D.S. Cordeiro	141 (1990) 379
Bianucci, M., M. Maestro and P. Walde, Bell-shaped curves of the enzyme activity in reverse micelles: a simplified model for hydrolytic reactions	141 (1990) 273
Botschwina, P. and P. Sebald, Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN <sup>+</sup>	141 (1990) 311
Brudzynski, R.J., see R.J. Sension	141 (1990) 393
Chaffins, S.A., see B.E. Kahn	141 (1990) 21
Clavilier, J., K. El Achi and A. Rodes, In situ probing of step and terrace sites on Pt(S)-[ <i>n</i> (111)×(111)] electrodes	141 (1990) 1
Cook, J.P.D., R. Pascual, E. Weigold, W. von Niessen and P. Tomasello, An experimental and theoretical investigation of the valence orbital momentum distributions and binding energy spectra of nitrogen	141 (1990) 211
Cordeiro, M.N.D.S., J.A.N.F. Gomes, A. González-Lafont, J.M. Lluch and J. Bertrán, The role of many-body interactions in the stability of hydrated Cu <sup>2+</sup> clusters	141 (1990) 379
Costa, M., see A. Tadjeddine	141 (1990) 15
Dalton, E.F., N.A. Surridge, J.C. Jernigan, K.O. Wilbourn, J.S. Facci and R.W. Murray, Charge transport in electroactive polymers consisting of fixed molecular redox sites	141 (1990) 143
Daudey, J.-P., see M. Merchan	141 (1990) 285
De Almeida, W.B., An ab initio study of the CO <sub>2</sub> ...C <sub>2</sub> H <sub>2</sub> binary complex	141 (1990) 297
Dean, M.H., see P. Meisterjahn	141 (1990) 131
Eichberger, R. and F. Willig, Ultrafast electron injection from excited dye molecules into semiconductor electrodes	141 (1990) 159
El Achi, K., see J. Clavilier	141 (1990) 1
Facci, J.S., see E.F. Dalton	141 (1990) 143
Forstmann, F., see J.P. Badiali	141 (1990) 63
Frisch, M., M. Head-Gordon and J. Pople, Direct analytic SCF second derivatives and electric field properties	141 (1990) 189
García-Ayllón, A. and J. Santamaría, Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform	141 (1990) 197

Gomes, J.A.N.F., see M.N.D.S. Cordeiro	141 (1990) 379
González, M., see R. Sayós	141 (1990) 401
González-Lafont, A., see M.N.D.S. Cordeiro	141 (1990) 379
Gonzalez-Luque, R., see M. Merchan	141 (1990) 285
Gui, J.Y., see B.E. Kahn	141 (1990) 21
Head-Gordon, M., see M. Frisch	141 (1990) 189
Henderson, D., Explicit formulae for the ion and solvent profiles in the electric double layer using the mean spherical approximation	141 (1990) 79
Hopkirk, A., see I.C. Walker	141 (1990) 365
Hubbard, A.T., see B.E. Kahn	141 (1990) 21
Hudson, B.S., see R.J. Sension	141 (1990) 393
Imre, D.G., see R.J. Sension	141 (1990) 393
Jernigan, J.C., see E.F. Dalton	141 (1990) 143
Jewsbury, P. and K. Lawley, A model for the relative intensities among ion pair→valence transitions in the heavier halogens and rare gas halides	141 (1990) 225
Kahn, B.E., S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard, Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics	141 (1990) 21
Kannen, G. and A. Otto, Optical studies on the quenching of the SERS activity of silver electrodes	141 (1990) 51
Karpfen, A., see P.G. Szalay	141 (1990) 355
Kharkats, Yu.I. and J. Ulstrup, Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions	141 (1990) 117
Kharlamov, B.M., see N.I. Ulitsky	141 (1990) 441
Kido, H., see N. Mikami	141 (1990) 431
Kikuma, J., see H. Umemoto	141 (1990) 457
Kowalczyk, A., see O. Rolinski	141 (1990) 265
Lawley, K., see P. Jewsbury	141 (1990) 225
Lischka, H., see P.G. Szalay	141 (1990) 355
Lluch, J.M., see M.N.D.S. Cordeiro	141 (1990) 379
Lu, F., see B.E. Kahn	141 (1990) 21
Lund, A., see L. Sjöqvist	141 (1990) 417
Maestro, M., see M. Bianucci	141 (1990) 273
Marsden, C.J. and B.J. Smith, The harmonic force field and $r_z$ molecular structure of di-sulphur monoxide, $S_2O$	141 (1990) 325
Marsden, C.J. and B.J. Smith, An ab initio study of many isomers of $S_2O_2$ . A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO	141 (1990) 335
Masaki, A., see H. Umemoto	141 (1990) 457
Meisterjahn, P., J.W. Schultze, B. Siemensmeyer, U. Stimming and M.H. Dean, Electron transfer reactions on passive iron electrodes	141 (1990) 131

- Merchan, M., J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil, Analysis of the CIPSI/DCCI approach to characterize the HF and F<sub>2</sub> single bond 141 (1990) 285
- Mikami, N., R. Ohki and H. Kido, Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization 141 (1990) 431
- Mulder, W.H. and J.H. Sluyters, The impedance of a plane electrode with a circular electro-active area both in the ideally polarized and the activation-controlled case 141 (1990) 105
- Murray, R.W., see E.F. Dalton 141 (1990) 143
- Nebot-Gil, I., see M. Merchan 141 (1990) 285
- Nordholm, S. and M.G. Sceats, The reduction of dissociation/recombination theory to one-dimensional form 141 (1990) 261
- Ohki, R., see N. Mikami 141 (1990) 431
- Otto, A., see G. Kannen 141 (1990) 51
- Palmer, M.H., see I.C. Walker 141 (1990) 365
- Pascual, R., see J.P.D. Cook 141 (1990) 211
- Personov, R.I., see N.I. Ulitsky 141 (1990) 441
- Pons, S., see A.E. Russell 141 (1990) 41
- Pople, J., see M. Frisch 141 (1990) 189
- Rahmani, A., see A. Tadjeddine 141 (1990) 15
- Richmond, G.L., see J.M. Robinson 141 (1990) 175
- Robinson, J.M. and G.L. Richmond, Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation 141 (1990) 175
- Rodes, A., see J. Clavilier 141 (1990) 1
- Rolinski, O., A. Balter and A. Kowalczyk, Fluorescence decay of solvated polar molecules in an electric field 141 (1990) 265
- Russell, A.E., S. Pons and M.R. Anderson, Infrared spectroelectrochemical measurements of the electrochemical double layer: using carbon monoxide as a double layer probe molecule 141 (1990) 41
- Santamaría, J., see A. García-Ayllón 141 (1990) 197
- Sato, S., see H. Umemoto 141 (1990) 457
- Sayós, R., M. González and A. Aguilar, Classical dynamics of the O(<sup>3</sup>P)+CS(X<sup>1</sup>Σ<sup>+</sup>)→CO(X<sup>1</sup>Σ<sup>+</sup>)+S(<sup>3</sup>P) reaction on the ground triplet potential energy surface 141 (1990) 401
- Sceats, M.G., see S. Nordholm 141 (1990) 261
- Schmickler, W., A model for the adsorption of metal ions on single crystal surfaces 141 (1990) 95
- Schultze, J.W., see P. Meisterjahn 141 (1990) 131
- Sebald, P., see P. Botschwina 141 (1990) 311
- Sension, R.J., R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre, Resonance emission studies of the photodissociating water molecule 141 (1990) 393
- Shiotani, M., see L. Sjöqvist 141 (1990) 417
- Shu, L. and G.J. Small, On the mechanism of nonphotochemical hole burning of optical transitions in amorphous solids 141 (1990) 447
- Siemensmeyer, B., see P. Meisterjahn 141 (1990) 131

- Sjöqvist, L., M. Shiotani and A. Lund, The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: an ESR and MNDO/AM1 study 141 (1990) 417
- Sluyters, J.H., see W.H. Mulder 141 (1990) 105
- Small, G.J., see L. Shu 141 (1990) 447
- Smith, B.J., see C.J. Marsden 141 (1990) 325
- Smith, B.J., see C.J. Marsden 141 (1990) 335
- Spoehr, E., Computer simulation of the water/platinum interface. Dynamical results 141 (1990) 87
- Stern, D.A., see B.E. Kahn 141 (1990) 21
- Stimming, U., see P. Meisterjahn 141 (1990) 131
- Surridge, N.A., see E.F. Dalton 141 (1990) 143
- Szalay, P.G., A. Karpfen and H. Lischka, Geometry relaxation effects in the  $1^1\text{B}_2$  and  $2^1\text{A}_1$  states of cis-1,3-butadiene 141 (1990) 355
- Tadjeddine, A., A. Rahmani and M. Costa, Optical behavior of liquid mercury-electrolyte interface studied by surface plasmon excitation 141 (1990) 15
- Tomasello, P., see J.P.D. Cook 141 (1990) 211
- Ulitsky, N.I., B.M. Kharlamov and R.I. Personov, Effect of a high magnetic field on the degenerate S-S transitions of organic molecules in amorphous matrices via hole burning: Zn-phthalocyanine in polyvinylbutyral 141 (1990) 441
- Ulstrup, J., see Yu.I. Kharkats 141 (1990) 117
- Umemoto, H., A. Masaki, J. Kikuma and S. Sato, The energy pooling processes between  $\text{Zn}(4^3\text{P}_J)$  atoms 141 (1990) 457
- Von Niessen, W., see J.P.D. Cook 141 (1990) 211
- Walde, P., see M. Bianucci 141 (1990) 273
- Walker, I.C., M.H. Palmer and A. Hopkirk, The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations 141 (1990) 365
- Wallace, R., The torsional energy levels of ethylene: interpretation in terms of two internal modes 141 (1990) 241
- Weigold, E., see J.P.D. Cook 141 (1990) 211
- Wilbourn, K.O., see E.F. Dalton 141 (1990) 143
- Willig, F., see R. Eichberger 141 (1990) 159
- Zhang, J., see R.J. Sension 141 (1990) 393

## LIST OF SUBJECTS

### 1 METHODS

#### 1.1 Theoretical

- 1.1.1 Group theory and algebras
- 1.1.2 Classical mechanics \*
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches \*
- 1.1.5 Coupling schemes and perturbative treatments \*
- 1.1.6 Relativistic quantum mechanics
- 1.1.7 Transport quantum mechanics \*
- 1.1.8 Equilibrium statistical mechanics \*
- 1.1.9 Statistical mechanics of stationary states
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories \*
- 1.1.11 Ab initio schemes for stationary properties \*
- 1.1.12 Computational and simulation methods \*
- 1.1.13 Molecular dynamics and scattering theory \*

#### 1.2 Experimental

- 1.2.1 Magnetic resonances \*
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy \*
- 1.2.4 Infrared spectroscopy \*
- 1.2.5 Raman spectroscopy \*
- 1.2.6 Visible and UV spectroscopy \*
- 1.2.7 Fluorescence spectroscopy \*
- 1.2.8 Photoelectron and Auger spectroscopy
- 1.2.9 X-ray spectroscopy
- 1.2.10 Electron impact spectroscopy \*
- 1.2.11 Laser methods \*
- 1.2.12 Picosecond spectroscopy \*
- 1.2.13 Non-linear optical spectroscopy \*
- 1.2.14 Synchrotron spectroscopies \*
- 1.2.15 Coherent optical spectroscopy
- 1.2.16 Optical pumping
- 1.2.17 Multiple resonance spectroscopy \*
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques
- 1.2.20 Time-resolved experiments \*
- 1.2.21 Mass spectrometry \*
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization
- 1.2.28 Measurement of macroscopic variables \*

### 2 OBJECTS

#### 2.1 Bulk systems

- 2.1.1 Gases \*
- 2.1.2 Supersonic beams \*
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions \*
- 2.1.5 Crystals \*
- 2.1.5.1 neat
- 2.1.5.2 mixed
- 2.1.6 Glasses
- 2.1.7 Liquid crystals
- 2.1.8 Polymers \*
- 2.1.9 Semiconductors \*
- 2.1.10 Metals and alloys \*
- 2.1.11 Thin films \*
- 2.1.12 Surfaces \*
- 2.1.13 Low-dimensional materials
- 2.1.14 Dielectrics \*
- 2.1.15 Plasmas
- 2.1.16 Biological systems \*

#### 2.2 Microscopic systems

- 2.2.1 Atoms \*
- 2.2.2 Molecules (neutral and ionic) \*
- 2.2.2.1 diatomic \*
- 2.2.2.2 small polyatomics \*
- 2.2.2.3 aromatics
- 2.2.2.4 other large \*
- 2.2.2.5 polymeric and biological
- 2.2.3 Molecular aggregates \*
- 2.2.3.1 dimers
- 2.2.3.2 van der Waals molecules
- 2.2.3.3 clusters \*
- 2.2.3.4 complexes \*
- 2.2.4 Free radicals (including hydronium and muonium) \*
- 2.2.5 Quasiparticles (including excitons)
- 2.2.6 Defects and impurities
- 2.2.7 Ions and charge carriers \*

\* Denotes subjects covered in this volume

### 3 PHENOMENA

- |        |   |        |  |
|--------|---|--------|--|
| 3.1    | Molecular structure *   | 3.16   | Multiphoton phenomena *                  |
| 3.2    | Vibrations and rotations of molecules *                                     | 3.17   | Reactions (including dissociation) *     |
| 3.3    | Electronic structure and states *   | 3.17.1 | gas phase *                              |
| 3.4    | Electric and magnetic properties *  | 3.17.2 | condensed phase *                        |
| 3.5    | Spin splittings   | 3.17.3 | photochemical                            |
| 3.6    | Optical activity  | 3.18   | Tunnelling *                             |
| 3.7    | Molecular interactions *  | 3.19   | Electron transfer *                      |
| 3.8    | Spectral bandshapes and intensities *                                       | 3.20   | Positron annihilation                    |
| 3.9    | Coupling of electronic and nuclear motion *                                 | 3.21   | Ionization (including Rydberg states) *  |
| 3.10   | Energy transfer processes *   | 3.22   | Molecular motion (including diffusive) * |
| 3.11   | Molecular photophysical processes *   | 3.23   | Isotopic effects                         |
| 3.12   | Intramolecular dynamics *   | 3.24   | Fluctuations and noise                   |
| 3.12.1 | radiationless transitions *   | 3.25   | Collective motion and excitations        |
| 3.12.2 | vibrational energy redistribution (including<br>vibrational dissociation) * | 3.26   | Surface effects and catalysis *          |
| 3.13   | Luminescence spectra, yields and lifetimes                                  | 3.27   | Thermodynamic and transport properties * |
| 3.14   | Coherence loss processes  | 3.28   | Structure of solids and liquids *        |
| 3.15   | Non-linear responses (including optical) *                                  | 3.29   | Critical phenomena                       |
|        |   | 3.30   | Phase transitions                        |

**SUBJECT INDEX TO VOLUME 141****METHODS****Theoretical***Classical mechanics*

Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform, A. García-Ayllón and J. Santamaría

141 (1990) 197

*Many body and quasiparticle approaches*

A model for the adsorption of metal ions on single crystal surfaces, W. Schmickler

An experimental and theoretical investigation of the valence orbital momentum distributions and binding energy spectra of nitrogen, J.P.D. Cook, R. Pascual, E. Weigold, W. von Niessen and P. Tomasello

141 (1990) 95

141 (1990) 211

*Coupling schemes and perturbative treatments*

A model for the relative intensities among ion pair→valence transitions in the heavier halogens and rare gas halides, P. Jewsbury and K. Lawley

The torsional energy levels of ethylene: interpretation in terms of two internal modes, R. Wallace

141 (1990) 225

141 (1990) 241

*Transport quantum mechanics*

Effective two-level reduction of *N*-level system dissipative quantum dynamics, P. Baňacký

141 (1990) 249

*Equilibrium statistical mechanics*

Long-range correlation between polar molecules adsorbed onto a dielectric solid, J.P. Badiali and F. Forstmann

Explicit formulae for the ion and solvent profiles in the electric double layer using the mean spherical approximation, D. Henderson

141 (1990) 63

141 (1990) 79

*Non-equilibrium thermodynamic and hydrodynamic theories*

Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup

The reduction of dissociation/recombination theory to one-dimensional form, S. Nordholm and M.G. Sceats

Fluorescence decay of solvated polar molecules in an electric field, O. Rolinski, A. Balter and A. Kowalczyk

Bell-shaped curves of the enzyme activity in reverse micelles: a simplified model for hydrolytic reactions, M. Bianucci, M. Maestro and P. Walde

141 (1990) 117

141 (1990) 261

141 (1990) 265

141 (1990) 273

*Ab initio schemes for stationary properties*

- Direct analytic SCF second derivatives and electric field properties, M. Frisch, M. Head-Gordon and J. Pople 141 (1990) 189
- The torsional energy levels of ethylene: interpretation in terms of two internal modes, R. Wallace 141 (1990) 241
- Analysis of the CIPSI/DCCI approach to characterize the HF and F<sub>2</sub> single bond, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil 141 (1990) 285
- An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida 141 (1990) 297
- Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN<sup>+</sup>, P. Botschwina and P. Sebald 141 (1990) 311
- The harmonic force field and *r*<sub>z</sub> molecular structure of disulphur monoxide, S<sub>2</sub>O, C.J. Marsden and B.J. Smith 141 (1990) 325
- An ab initio study of many isomers of S<sub>2</sub>O<sub>2</sub>. A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO, C.J. Marsden and B.J. Smith 141 (1990) 335
- Geometry relaxation effects in the 1<sup>1</sup>B<sub>2</sub> and 2<sup>1</sup>A<sub>1</sub> states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka 141 (1990) 355
- The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and A. Hopkirk 141 (1990) 365
- The role of many-body interactions in the stability of hydrated Cu<sup>2+</sup> clusters, M.N.D.S. Cordeiro, J.A.N.F. Gomes, A. González-Lafont, J.M. Lluch and J. Bertrán 141 (1990) 379

*Computational and simulation methods*

- Computer simulation of the water/platinum interface. Dynamical results, E. Spohr 141 (1990) 87
- The impedance of a plane electrode with a circular electro-active area both in the ideally polarized and the activation-controlled case, W.H. Mulder and J.H. Sluyters 141 (1990) 105
- Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform, A. García-Ayllón and J. Santamaría 141 (1990) 197
- An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida 141 (1990) 297
- The role of many-body interactions in the stability of hydrated Cu<sup>2+</sup> clusters, M.N.D.S. Cordeiro, J.A.N.F. Gomes, A. González-Lafont, J.M. Lluch and J. Bertrán 141 (1990) 379
- Resonance emission studies of the photodissociating water molecule, R.J. Sension, R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre 141 (1990) 393
- Classical dynamics of the O(<sup>3</sup>P) + CS(X<sup>1</sup>Σ<sup>+</sup>) → CO(X<sup>1</sup>Σ<sup>+</sup>) + S(<sup>3</sup>P) reaction on the ground triplet potential energy surface, R. Sayós, M. González and A. Aguilar 141 (1990) 401

*Molecular dynamics and scattering theory*

- Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform, A. García-Ayllón and J. Santamaría 141 (1990) 197
- Effective two-level reduction of *N*-level system dissipative quantum dynamics, P. Baňácký 141 (1990) 249
- Resonance emission studies of the photodissociating water molecule, R.J. Sension, R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre 141 (1990) 393
- Classical dynamics of the O(<sup>3</sup>P) + CS(X<sup>1</sup>Σ<sup>+</sup>) → CO(X<sup>1</sup>Σ<sup>+</sup>) + S(<sup>3</sup>P) reaction on the ground triplet potential energy surface, R. Sayós, M. González and A. Aguilar 141 (1990) 401

**Experimental***Magnetic resonances*

The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: an ESR and MNDO/AM1 study, L. Sjöqvist, M. Shiotani and A. Lund

141 (1990) 417

*Microwave spectroscopy*

The harmonic force field and  $r_z$  molecular structure of disulphur monoxide,  $S_2O$ , C.J. Marsden and B.J. Smith

141 (1990) 325

An ab initio study of many isomers of  $S_2O_2$ . A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO, C.J. Marsden and B.J. Smith

141 (1990) 335

*Infrared spectroscopy*

Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics, B.E. Kahn, S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard

141 (1990) 21

The harmonic force field and  $r_z$  molecular structure of disulphur monoxide,  $S_2O$ , C.J. Marsden and B.J. Smith

141 (1990) 325

*Raman spectroscopy*

Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics, B.E. Kahn, S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard

141 (1990) 21

Optical studies on the quenching of the SERS activity of silver electrodes, G. Kannen and A. Otto

141 (1990) 51

Resonance emission studies of the photodissociating water molecule, R.J. Sension, R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre

141 (1990) 393

*Visible and UV spectroscopy*

Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido

141 (1990) 431

Effect of a high magnetic field on the degenerate S-S transitions of organic molecules in amorphous matrices via hole burning: Zn-phthalocyanine in polyvinylbutyral, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov

141 (1990) 441

*Fluorescence spectroscopy*

Ultrafast electron injection from excited dye molecules into semiconductor electrodes, R. Eichberger and F. Willig

141 (1990) 159

A model for the relative intensities among ion pair→valence transitions in the heavier halogens and rare gas halides, P. Jewsbury and K. Lawley

141 (1990) 225

Fluorescence decay of solvated polar molecules in an electric field, O. Rolinski, A. Balter and A. Kowalczyk

141 (1990) 265

*Electron impact spectroscopy*

Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics, B.E. Kahn, S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard

141 (1990) 21

An experimental and theoretical investigation of the valence orbital momentum distributions and binding energy spectra of nitrogen, J.P.D. Cook, R. Pascual, E. Weigold, W. von Niessen and P. Tomasello

141 (1990) 211

The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and A. Hopkirk

141 (1990) 365

*Laser methods*

Resonance emission studies of the photodissociating water molecule, R.J. Sensen, R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre

141 (1990) 393

Effect of a high magnetic field on the degenerate S-S transitions of organic molecules in amorphous matrices via hole burning: Zn-phthalocyanine in polyvinylbutyral, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov

141 (1990) 441

On the mechanism of nonphotochemical hole burning of optical transitions in amorphous solids, L. Shu and G.J. Small

141 (1990) 447

*Picosecond spectroscopy*

Ultrafast electron injection from excited dye molecules into semiconductor electrodes, R. Eichberger and F. Willig

141 (1990) 159

*Non-linear optical spectroscopy*

On the mechanism of nonphotochemical hole burning of optical transitions in amorphous solids, L. Shu and G.J. Small

141 (1990) 447

*Synchrotron spectroscopies*

The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and A. Hopkirk

141 (1990) 365

*Multiple resonance spectroscopy*

Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido

141 (1990) 431

*Time-resolved experiments*

Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond

141 (1990) 175

The energy pooling processes between Zn( $4^3P_J$ ) atoms, H. Umemoto, A. Masaki, J. Kikuma and S. Sato

141 (1990) 457

*Mass spectrometry*

Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido

141 (1990) 431

*Measurement of macroscopic variables*

- In situ probing of step and terrace sites on Pt(S)-[ $n(111)\times(111)$ ] electrodes, J. Clavilier, K. El Achi and A. Rodes 141 (1990) 1  
 The impedance of a plane electrode with a circular electro-active area both in the ideally polarized and the activation-controlled case, W.H. Mulder and J.H. Sluyters 141 (1990) 105  
 Electron transfer reactions on passive iron electrodes, P. Meisterjahn, J.W. Schultze, B. Siemensmeyer, U. Stimming and M.H. Dean 141 (1990) 131

**OBJECTS****Bulk systems***Gases*

- The energy pooling processes between Zn( $4^3P_J$ ) atoms, H. Umemoto, A. Masaki, J. Kikuma and S. Sato 141 (1990) 457

*Supersonic beams*

- Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido 141 (1990) 431

*Liquid mixtures and solutions*

- Fluorescence decay of solvated polar molecules in an electric field, O. Rolinski, A. Balter and A. Kowalczyk 141 (1990) 265

*Crystals*

- A model for the adsorption of metal ions on single crystal surfaces, W. Schmickler 141 (1990) 95

*Polymers*

- Charge transport in electroactive polymers consisting of fixed molecular redox sites, E.F. Dalton, N.A. Surridge, J.C. Jernigan, K.O. Wilbourn, J.S. Facci and R.W. Murray 141 (1990) 143

*Semiconductors*

- Ultrafast electron injection from excited dye molecules into semiconductor electrodes, R. Eichberger and F. Willig 141 (1990) 159

*Metals and alloys*

- A model for the adsorption of metal ions on single crystal surfaces, W. Schmickler 141 (1990) 95

*Thin films*

- A model for the adsorption of metal ions on single crystal surfaces, W. Schmickler 141 (1990) 95  
 Electron transfer reactions on passive iron electrodes, P. Meisterjahn, J.W. Schultze, B. Siemensmeyer, U. Stimming and M.H. Dean 141 (1990) 131

- Charge transport in electroactive polymers consisting of fixed molecular redox sites, E.F. Dalton, N.A. Surridge, J.C. Jernigan, K.O. Wilbourn, J.S. Facci and R.W. Murray 141 (1990) 143

- Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond 141 (1990) 175

*Surfaces*

- In situ probing of step and terrace sites on Pt(S)-[ $n(111) \times (111)$ ] electrodes, J. Clavilier, K. El Achi and A. Rodes 141 (1990) 1
- Optical behavior of liquid mercury-electrolyte interface studied by surface plasmon excitation, A. Tadjeddine, A. Rahmani and M. Costa 141 (1990) 15
- Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics, B.E. Kahn, S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard 141 (1990) 21
- Infrared spectroelectrochemical measurements of the electrochemical double layer: using carbon monoxide as a double layer probe molecule, A.E. Russell, S. Pons and M.R. Anderson 141 (1990) 41
- Optical studies on the quenching of the SERS activity of silver electrodes, G. Kannen and A. Otto 141 (1990) 51
- Long-range correlation between polar molecules adsorbed onto a dielectric solid, J.P. Badiali and F. Forstmann 141 (1990) 63
- Explicit formulae for the ion and solvent profiles in the electric double layer using the mean spherical approximation, D. Henderson 141 (1990) 79
- Computer simulation of the water/platinum interface. Dynamical results, E. Spohr 141 (1990) 87
- The impedance of a plane electrode with a circular electro-active area both in the ideally polarized and the activation-controlled case, W.H. Mulder and J.H. Sluyters 141 (1990) 105
- Ultrafast electron injection from excited dye molecules into semiconductor electrodes, R. Eichberger and F. Willig 141 (1990) 159
- Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond 141 (1990) 175

*Dielectrics*

- Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117

*Biological systems*

- Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117
- Bell-shaped curves of the enzyme activity in reverse micelles: a simplified model for hydrolytic reactions, M. Bianucci, M. Maestro and P. Walde 141 (1990) 273

*Microscopic systems**Atoms*

- The energy pooling processes between Zn( $4^3P_J$ ) atoms, H. Umemoto, A. Masaki, J. Kikuma and S. Sato 141 (1990) 457

*Molecules (neutral and ionic)*

- The reduction of dissociation/recombination theory to one-dimensional form, S. Nordholm and M.G. Sceats 141 (1990) 261
- Fluorescence decay of solvated polar molecules in an electric field, O. Rolinski, A. Balter and A. Kowalczyk 141 (1990) 265
- Geometry relaxation effects in the  $1^1B_2$  and  $2^1A_1$  states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka 141 (1990) 355

The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: an ESR and MNDO/AM1 study, L. Sjöqvist, M. Shiotani and A. Lund

141 (1990) 417

*-diatomic*

An experimental and theoretical investigation of the valence orbital momentum distributions and binding energy spectra of nitrogen, J.P.D. Cook, R. Pascual, E. Weigold, W. von Niessen and P. Tomasello

141 (1990) 211

A model for the relative intensities among ion pair→valence transitions in the heavier halogens and rare gas halides, P. Jewsbury and K. Lawley

141 (1990) 225

Analysis of the CIPSI/DCCI approach to characterize the HF and F<sub>2</sub> single bond, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil

141 (1990) 285

Classical dynamics of the O(<sup>3</sup>P) + CS(X<sup>1</sup>Σ<sup>+</sup>) → CO(X<sup>1</sup>Σ<sup>+</sup>) + S(<sup>3</sup>P) reaction on the ground triplet potential energy surface, R. Sayós, M. González and A. Aguilar

141 (1990) 401

*-small polyatomics*

Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform, A. García-Ayllón and J. Santamaría

141 (1990) 197

The torsional energy levels of ethylene: interpretation in terms of two internal modes, R. Wallace

141 (1990) 241

Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN<sup>+</sup>, P. Botschwina and P. Sebald

141 (1990) 311

Geometry relaxation effects in the 1<sup>1</sup>B<sub>2</sub> and 2<sup>1</sup>A<sub>1</sub> states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka

141 (1990) 355

The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and A. Hopkirk

141 (1990) 365

Resonance emission studies of the photodissociating water molecule, R.J. Sension, R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre

141 (1990) 393

*-other large*

Photodissociation of jet-cooled acetylacetato complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido

141 (1990) 431

Effect of a high magnetic field on the degenerate S-S transitions of organic molecules in amorphous matrices via hole burning: Zn-phthalocyanine in polyvinylbutyral, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov

141 (1990) 441

*Molecular aggregates*

Bell-shaped curves of the enzyme activity in reverse micelles: a simplified model for hydrolytic reactions, M. Bianucci, M. Maestro and P. Walde

141 (1990) 273

An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida

141 (1990) 297

*-clusters*

The role of many-body interactions in the stability of hydrated Cu<sup>2+</sup> clusters, M.N.D.S. Cordeiro, J.A.N.F. Gomes, A. González-Lafont, J.M. Lluch and J. Bertrán

141 (1990) 379

*-complexes*

Effective two-level reduction of *N*-level system dissipative quantum dynamics, P. Baňácký

141 (1990) 249

*Free radicals (including hydronium and muonium)*

The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: an ESR and MNDO/AM1 study, L. Sjöqvist, M. Shiotani and A. Lund

141 (1990) 417

*Ions and charge carriers*

Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond

141 (1990) 175

**PHENOMENA***Molecular structure*

Analysis of the CIPSI/DCCI approach to characterize the HF and F<sub>2</sub> single bond, M. Merchan, J.-P. Daudey, R. Gonzalez-Luque and I. Nebot-Gil

141 (1990) 285

An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida

141 (1990) 297

Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN<sup>+</sup>, P. Botschwina and P. Sebald

141 (1990) 311

The harmonic force field and *r*<sub>z</sub> molecular structure of disulphur monoxide, S<sub>2</sub>O, C.J. Marsden and B.J. Smith

141 (1990) 325

An ab initio study of many isomers of S<sub>2</sub>O<sub>2</sub>. A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO, C.J. Marsden and B.J. Smith

141 (1990) 335

Geometry relaxation effects in the 1<sup>1</sup>B<sub>2</sub> and 2<sup>1</sup>A<sub>1</sub> states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka

141 (1990) 355

The structure of trans- and cis-3-hexene radical cations stabilised in halocarbon matrices at low temperature: an ESR and MNDO/AM1 study, L. Sjöqvist, M. Shiotani and A. Lund

141 (1990) 417

*Vibrations and rotations of molecules*

The torsional energy levels of ethylene: interpretation in terms of two internal modes, R. Wallace

141 (1990) 241

An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida

141 (1990) 297

Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN<sup>+</sup>, P. Botschwina and P. Sebald

141 (1990) 311

The harmonic force field and *r*<sub>z</sub> molecular structure of disulphur monoxide, S<sub>2</sub>O, C.J. Marsden and B.J. Smith

141 (1990) 325

An ab initio study of many isomers of S<sub>2</sub>O<sub>2</sub>. A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO, C.J. Marsden and B.J. Smith

141 (1990) 335

*Electronic structure and states*

A model for the relative intensities among ion pair→valence transitions in the heavier halogens and rare gas halides, P. Jewsbury and K. Lawley

141 (1990) 225

An ab initio study of many isomers of S<sub>2</sub>O<sub>2</sub>. A combined theoretical and experimental analysis of the harmonic force field and molecular structure of cis-planar OSSO, C.J. Marsden and B.J. Smith

141 (1990) 335

Geometry relaxation effects in the 1<sup>1</sup>B<sub>2</sub> and 2<sup>1</sup>A<sub>1</sub> states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka

141 (1990) 355

- The electronic states of the azines. II. Pyridine, studied by VUV absorption, near-threshold electron energy loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker, M.H. Palmer and A. Hopkirk 141 (1990) 365
- Electric and magnetic properties*
- Effect of a high magnetic field on the degenerate S-S transitions of organic molecules in amorphous matrices via hole burning: Zn-phthalocyanine in polyvinylbutyral, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov 141 (1990) 441
- Molecular interactions*
- An ab initio study of the CO<sub>2</sub>...C<sub>2</sub>H<sub>2</sub> binary complex, W.B. De Almeida 141 (1990) 297
- Spectral bandshapes and intensities*
- Calculated spectroscopic properties for NCCN, CNCN, CNNC and HNCCN<sup>+</sup>, P. Botschwina and P. Sebald 141 (1990) 311
- Coupling of electronic and nuclear motion*
- Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117
- Energy transfer processes*
- The energy pooling processes between Zn(4<sup>3</sup>P<sub>J</sub>) atoms, H. Umemoto, A. Masaki, J. Kikuma and S. Sato 141 (1990) 457
- Molecular photophysical processes*
- Geometry relaxation effects in the 1<sup>1</sup>B<sub>2</sub> and 2<sup>1</sup>A<sub>1</sub> states of cis-1,3-butadiene, P.G. Szalay, A. Karpfen and H. Lischka 141 (1990) 355
- Intramolecular dynamics*
- Stretch-bend coupling effect on the intramolecular vibrational relaxation in a two-mode model of CH overtone excited fluoroform, A. García-Ayllón and J. Santamaría 141 (1990) 197
- radiationless transitions*
- Dielectric image effects in environmental reorganization free energies and inter-reactant work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117
- vibrational energy redistribution (including vibrational dissociation)*
- The torsional energy levels of ethylene: interpretation in terms of two internal modes, R. Wallace 141 (1990) 241
- Non-linear responses (including optical)*
- Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond 141 (1990) 175
- Effective two-level reduction of *N*-level system dissipative quantum dynamics, P. Baňacký 141 (1990) 249
- Multiphoton phenomena*
- Photodissociation of jet-cooled acetylacetone complexes of the first transition metals. Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido 141 (1990) 431

*Reactions (including dissociation)*

Photodissociation of jet-cooled acetylacetone complexes of the first transition metals.  
Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido 141 (1990) 431

*-gas phase*

Resonance emission studies of the photodissociating water molecule, R.J. Sension,  
R.J. Brudzynski, B.S. Hudson, J. Zhang and D.G. Imre 141 (1990) 393  
Classical dynamics of the  $O(^3P) + CS(X^1\Sigma^+) \rightarrow CO(X^1\Sigma^+) + S(^3P)$  reaction on the ground  
triplet potential energy surface, R. Sayós, M. González and A. Aguilar 141 (1990) 401

*-condensed phase*

The reduction of dissociation/recombination theory to one-dimensional form, S. Nordholm  
and M.G. Sceats 141 (1990) 261  
Bell-shaped curves of the enzyme activity in reverse micelles: a simplified model for hy-  
drolytic reactions, M. Bianucci, M. Maestro and P. Walde 141 (1990) 273

*Tunnelling*

Dielectric image effects in environmental reorganization free energies and inter-reactant  
work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117  
Electron transfer reactions on passive iron electrodes, P. Meisterjahn, J.W. Schultze,  
B. Siemensmeyer, U. Stimming and M.H. Dean 141 (1990) 131  
Effective two-level reduction of  $N$ -level system dissipative quantum dynamics, P. Baňacký 141 (1990) 249

*Electron transfer*

The impedance of a plane electrode with a circular electro-active area both in the ideally  
polarized and the activation-controlled case, W.H. Mulder and J.H. Sluyters 141 (1990) 105  
Dielectric image effects in environmental reorganization free energies and inter-reactant  
work terms of metalloprotein electron transfer reactions, Yu.I. Kharkats and J. Ulstrup 141 (1990) 117  
Electron transfer reactions on passive iron electrodes, P. Meisterjahn, J.W. Schultze,  
B. Siemensmeyer, U. Stimming and M.H. Dean 141 (1990) 131  
Charge transport in electroactive polymers consisting of fixed molecular redox sites,  
E.F. Dalton, N.A. Surridge, J.C. Jernigan, K.O. Wilbourn, J.S. Facci and R.W. Murray 141 (1990) 143  
Ultrafast electron injection from excited dye molecules into semiconductor electrodes,  
R. Eichberger and F. Willig 141 (1990) 159

*Ionization (including Rydberg states)*

An experimental and theoretical investigation of the valence orbital momentum distri-  
butions and binding energy spectra of nitrogen, J.P.D. Cook, R. Pascual, E. Weigold,  
W. von Niessen and P. Tomasello 141 (1990) 211  
Photodissociation of jet-cooled acetylacetone complexes of the first transition metals.  
Free metal generation and fragmentational ionization, N. Mikami, R. Ohki and H. Kido 141 (1990) 431

*Molecular motion (including diffusive)*

Computer simulation of the water/platinum interface. Dynamical results, E. Spohr 141 (1990) 87  
The reduction of dissociation/recombination theory to one-dimensional form, S. Nordholm  
and M.G. Sceats 141 (1990) 261  
Fluorescence decay of solvated polar molecules in an electric field, O. Rolinski, A. Balter  
and A. Kowalczyk 141 (1990) 265

*Surface effects and catalysis*

- In situ probing of step and terrace sites on Pt(S)-[ $n(111)\times(111)$ ] electrodes, J. Clavilier, K. El Achi and A. Rodes 141 (1990) 1
- In situ probing of step and terrace sites on Pt(S)-[ $n(111)\times(111)$ ] electrodes, J. Clavilier, K. El Achi and A. Rodes 141 (1990) 1
- Optical behavior of liquid mercury-electrolyte interface studied by surface plasmon excitation, A. Tadjeddine, A. Rahmani and M. Costa 141 (1990) 15
- Surface vibrational spectroscopy. A comparison of the EELS spectra of organic adsorbates at Pt(111) with IR and Raman spectra of the unadsorbed organics, B.E. Kahn, S.A. Chaffins, J.Y. Gui, F. Lu, D.A. Stern and A.T. Hubbard 141 (1990) 21
- Infrared spectroelectrochemical measurements of the electrochemical double layer: using carbon monoxide as a double layer probe molecule, A.E. Russell, S. Pons and M.R. Anderson 141 (1990) 41
- Optical studies on the quenching of the SERS activity of silver electrodes, G. Kannen and A. Otto 141 (1990) 51
- Long-range correlation between polar molecules adsorbed onto a dielectric solid, J.P. Badiali and F. Forstmann 141 (1990) 63
- Computer simulation of the water/platinum interface. Dynamical results, E. Spohr 141 (1990) 87
- A model for the adsorption of metal ions on single crystal surfaces, W. Schmickler 141 (1990) 95
- Time-resolved measurements of the electrodeposition of thallium on silver electrodes by optical second-harmonic generation, J.M. Robinson and G.L. Richmond 141 (1990) 175

*Thermodynamic and transport properties*

- Charge transport in electroactive polymers consisting of fixed molecular redox sites, E.F. Dalton, N.A. Surridge, J.C. Jernigan, K.O. Wilbourn, J.S. Facci and R.W. Murray 141 (1990) 143

*Structure of solids and liquids*

- Explicit formulae for the ion and solvent profiles in the electric double layer using the mean spherical approximation, D. Henderson 141 (1990) 79

